

NASA TM X-55585

# OSCILLATOR STRENGTHS FOR RESONANCE LINES OF IONS IN THE NEON ISOELECTRIC SEQUENCE

BY

S. O. KASTNER

K. OMIDVAR

J. H. UNDERWOOD

JUNE 1966



**GODDARD SPACE FLIGHT CENTER**  
**GREENBELT, MD.**

GPO PRICE \$ \_\_\_\_\_

CFSTI PRICE(S) \$ \_\_\_\_\_

Hard copy (HC) 1.00Microfiche (MF) 150**N67 13227**

(ACCESSION NUMBER)

18  
(PAGES)TMX-55585  
(NASA CR OR TMX OR AD NUMBER)

(THRU)

(CODE)

24  
(CATEGORY)

FACILITY FORM 602

OSCILLATOR STRENGTHS FOR RESONANCE LINES  
OF IONS IN THE NEON ISOELECTRONIC SEQUENCE

S.O. KASTNER, K. OMIDVAR, J.H. UNDERWOOD

GODDARD SPACE FLIGHT CENTER  
GREENBELT, MARYLAND

## INTRODUCTION

We give oscillator strengths in Table 2 for some extreme ultraviolet resonance lines of ionized atoms in the neon isoelectronic sequence, up to Fe XVII. The last ion motivated the work, since its lines have been recently observed in the coronal spectrum by Blake et al<sup>1</sup> and by workers in this laboratory; knowledge of the oscillator strengths of these lines should permit estimates of the electron density and temperature of the emitting regions to be made.\*

## CALCULATION

A computer program of C. Froese<sup>2</sup> was used, which calculates Hartree-Fock wave functions for an isoelectronic sequence and uses these to form Slater integrals  $F^k$ ,  $G^k$  and the spin-orbit parameter  $\zeta l$ . The secular equations involving these parameters, for the  $J=1$  levels of the  $2p^5 3s$  and  $2p^5 3d$  configurations, are respectively quadratic and cubic; these were solved to give intermediate-coupling coefficients<sup>3</sup> for the Hartree-Fock (LS) wave functions. Electric dipole length radial integrals were formed between the  $^1P$  wave functions of the excited configurations and the  $^1S$  wave function of the ground state. Oscillator strengths were then calculated using the line strength formula for  $p^n - p^{n-1}l$  given by Shore and Menzel in their general tables<sup>4</sup>. This formula takes into account the fact that any one of the six equivalent  $p$  electrons in the outer shell may contribute to the transition. Observed energies<sup>4</sup> were used except in the cases of  $V^{+13}$  and  $A^{+8}$  whose energies were interpolated between those of neighboring members of the sequence.

\* R. H. Garstang (private communication) has also calculated oscillator strengths for the Fe XVII transitions. The values reported here are in general agreement with his.

We find that for ions Al IV to Fe XVII the designation of the  $2p^5 3d - {}^1P_1$  and  $2p^5 3d - {}^3D_1$  levels in AEL<sup>5</sup> should be interchanged, to reflect the respective amounts of  ${}^1P_1$  and  ${}^3D_1$  character in their actual wave functions; for Fe XVII and Cl VIII the coefficients of  ${}^1P$  component in the three levels are (using AEL designations):

TABLE 1

	${}^3P_1$	${}^3D_1$	${}^1P_1$
Fe XVII	0.19	0.83	0.45
Cl VIII	0.095	0.95	0.30

The original assignment of these levels by Soderqvist<sup>6</sup> and others was probably based on parentage<sup>7</sup>, the parents of the  ${}^3D$  and  ${}^1P$  terms being respectively the  ${}^2P_{1/2}$  and  ${}^2P_{3/2}$  terms of the  $2p^5$  core which are split by the spin-orbit interaction. However, since the electrostatic interactions are greater in magnitude than the spin-orbit interactions for the more highly ionized atoms of the sequence, parentage is not the determining factor for these ions.

In Table 2 and in what follows we use the suggested change in notation, though of course, LS coupling notation cannot fully describe these levels.

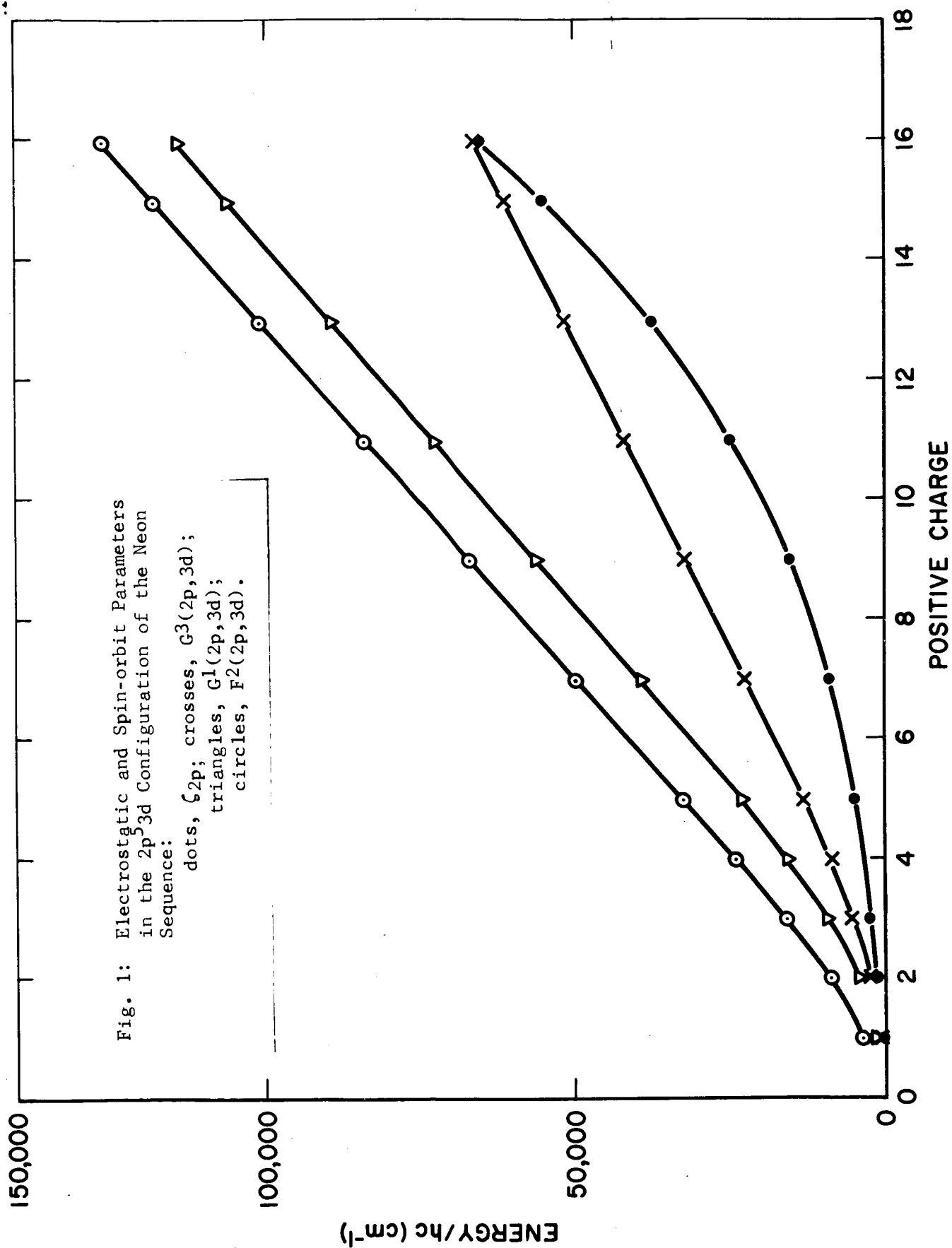
TABLE 2

TRANSITION ION	$2p^5 3s - 2p^6$		$2p^5 3d - 2p^6$		
	$^1P_1 - ^1S_0$	$^3P_1 - ^1S_0$	$^1P_1 - ^1S_0$	$^3D_1 - ^1S_0$	$^3P_1 - ^1S_0$
Fe XVII	0.070	0.082	2.24	0.57	0.097
Mn XVI	0.074	0.081	2.22	0.52	0.082
Cr XV	0.080	0.079	2.24	0.44	0.069
V XIV	0.085	0.078	2.22	0.38	0.056
Ti XIII	0.092	0.075	2.19	0.33	0.046
Sc XII	0.10	0.071	2.12	0.28	0.037
Ca XI	0.11	0.066	2.05	0.24	0.030
K X	0.12	0.060	1.94	0.20	0.024
A IX	0.14	0.052	1.81	0.18	0.019
Cl VIII	0.15	0.044	1.62	0.16	0.016
S VII	0.17	0.036	1.42	0.15	0.013
P VI	0.18	0.028	1.15	0.16	0.012
Si V	0.19	0.021	0.84	0.19	0.011
Al IV	0.20	0.015	0.48	0.25	0.011
Mg III	0.21	0.011	0.16	0.26	0.010
Na II	0.19	0.0093	0.039	0.12	0.0077

The behaviour of the triplet as the degree of ionization increases along the sequence depends (subject to remarks below on the comparison with observation) on the relative values of the electrostatic and spin-orbit parameters illustrated in Figure 1. For neutral neon the spin-orbit parameter  $\zeta_{2p}$  is substantially larger than the electrostatic parameters, so that pair coupling applies. With moderate degrees of ionization, however, the situation is reversed so that approximate LS coupling holds and one transition is more intense than the others. It is interesting to note that because of the increasing slope of the curve for  $\zeta_{2p}$ , it must eventually again become larger than the electrostatic parameters for ions in the sequence past Fe XVII, so that pair coupling will again hold.

#### COMPARISON WITH OTHER CALCULATIONS AND OBSERVATIONS

There is a great scarcity of oscillator strengths for ions in the neon sequence, except for neon itself, as seen from the bibliography of Glennon and Wiese<sup>8</sup>. Peterson<sup>9</sup> has calculated the ratio of oscillator strengths for the  $2p^5 3s$  ( $^3P_1$ ,  $^1P_1$ ) -  $2p^6$  ( $^1S_0$ ) doublet of Na II as 21.0, derived from the observed energy levels. The corresponding result from Table 2 is 21.0 also, as expected since the same levels were used. Mendel'stam<sup>10</sup> gives LS coupling oscillator strengths for the transitions  $2p^5 3s$  -  $2p^6$  and  $2p^5 3d$  -  $2p^6$  of Fe XVII as being 0.024 and 0.524 respectively. Though he does not give the source of these values, they appear to be one-electron oscillator strengths; when multiplied by six they become 0.144 and 3.14, comparing well with the corresponding  $\Sigma gf = 0.152$  and 2.91 from Table 2. Comparisons with other calculations, however, do not answer the



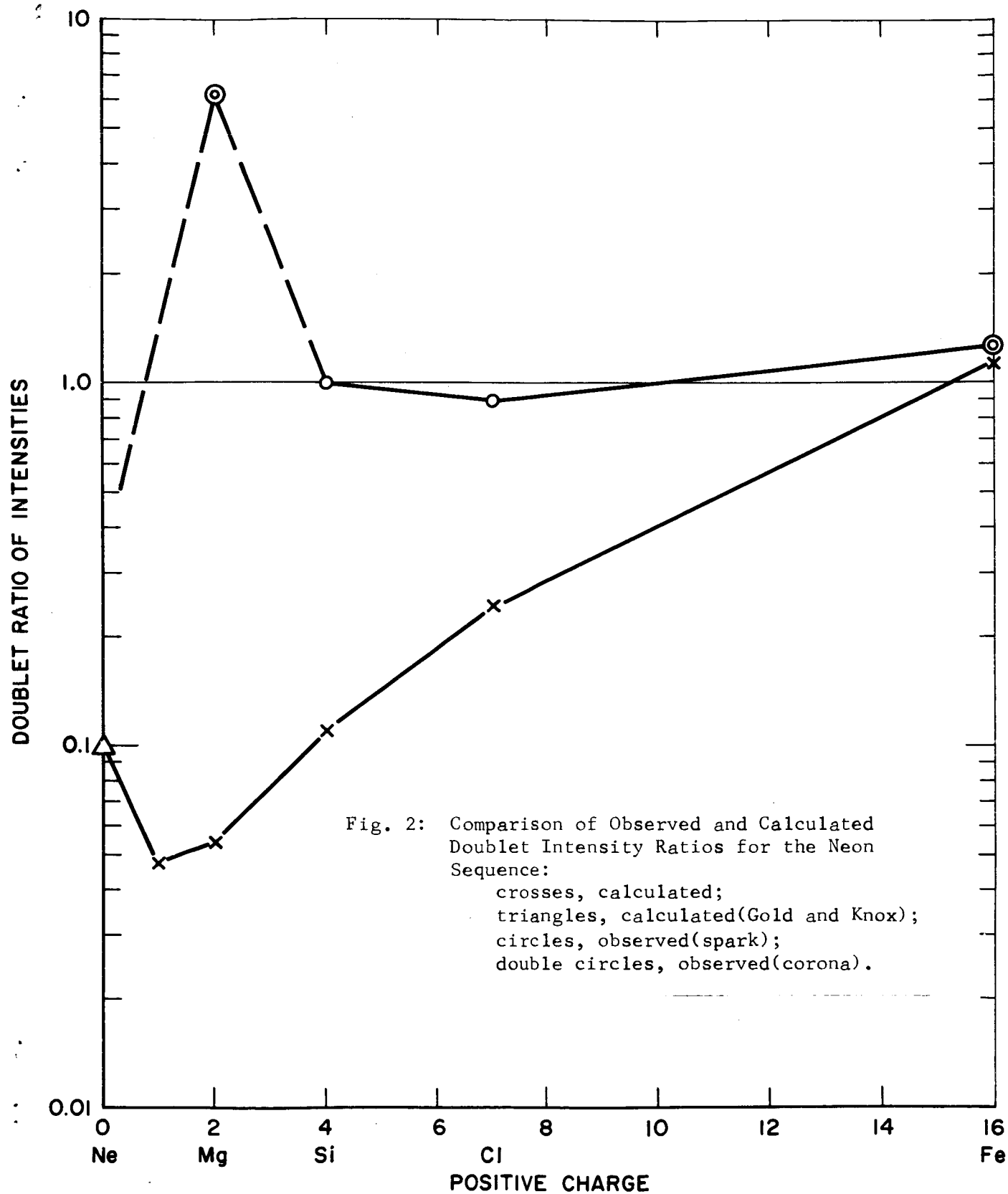
important question of how well the results agree with observation. The situation is less satisfactory in this regard, as discussed next.

In Table 3 are listed the few available observed ratios of intensities for the resonance lines, the intensity for ( $^1P_1 - ^1S_0$ ) being taken as unity in each case.

TABLE 3

TRANSITION ION	$2p^5 3s - 2p^6$		$2p^5 3d - 2p^6$		
	$^1P_1 - ^1S_0$	$^3P_1 - ^1S_0$	$^1P_1 - ^1S_0$	$^3D_1 - ^1S_0$	$^3P_1 - ^1S_0$
Fe XVII	1.0	1.28	1.0	0.62	-
Cl VIII	1.0	0.9	1.0	0.71	0.29
Si V	1.0	1.0	1.0	0.67	0.13
Mg III	1.0	6.3	-	-	-

The intensities for Cl VIII are given by Edlen<sup>11</sup>, those for Si V by Ferner<sup>12</sup>, the sources in both cases being sparks. The intensities of the Fe XVII lines are taken from Blake et al<sup>1</sup>, as observed in the corona, while the Mg III lines have been tentatively identified in the corona by Pecker and Rohrllich<sup>13</sup> and by Jordan<sup>14</sup>. In spite of the meagerness of this data and the variation in excitation conditions, it is felt to be of interest to plot the doublet ratios in Figure 2 together with our calculated ratios



and the value of Gold and Knox<sup>15</sup> for neon. A zero ordinate in the figure would signify pure LS coupling. The curve through the value for Mg III is drawn as a dashed line to emphasize its complete uncertainty. No direct experimental measurement of the neon doublet ratio is available but the  $f$  value for the singlet transition has been measured by Korolev et al<sup>16</sup> to be 0.16, in rough agreement with Gold and Knox's value of 0.11. This implies approximate LS coupling, so that the observed curve must descend from Mg III (or Na II) to the vicinity of the calculated curve, as indicated.

If we assume that in both the spark sources and the corona (a) the population of the upper levels takes place mainly by collisional excitation, and (b) the optical depths in the lines are small, assumptions which are most probably valid for the corona but less certainly so for the sparks, then we may infer from the figure that the disagreement between observation and the present calculation is greatest for the ions immediately beyond neon, becoming less for the more highly ionized members of the sequence. The disagreement may be due to the effects of configuration interaction.

In the case of the triplet, also, agreement is best for Fe XVII and becomes poorer for decreasing ionization though there are still fewer observations on which to base this statement. The higher relative coronal intensity for the  $^3D_1 - ^1S_0$  transition in Fe XVII may possibly represent the effect of appreciable optical depth.

More experimental measurements for ions of the neon sequence would put Figure 2 and the above comments on firmer ground.

## CONCLUSIONS

The single configuration treatment with intermediate coupling gives oscillator strengths that agree fairly well with observed intensity ratios in the case of Fe XVII, in the corona. Disagreement is marked, however, with the few observations of earlier ions in the neon sequence. If the comparison is meaningful, configuration interaction may be responsible.

## ACKNOWLEDGEMENT

We wish to thank Dr. C. Froese for advice on her program as well as B. Phillips and C. Wade for assistance with computer programming.

## REFERENCES

1. Blake, Chubb, Friedman, Unzicker - Astrophysical Journal 142, 1 (1965).
2. Froese, C. - Canadian Journal of Physics 41, 1895 (1963).
3. Condon and Shortley - Theory of Atomic Spectra, Cambridge University Press, 1953, Chapter XI.
4. Shore, B. W. and D. Menzel - Astrophys. Journal Supplement No. 106, 12, 187 (1965).
5. Sitterly, C.E. Moore - "Atomic Energy Levels", Natl. Bur. Stds. Circular 467, Washington, D. C.; Vols. 1(1949) and 2(1952).
6. Soderqvist - Nova Acta Reg. Soc. Sci. Uppsala (IV) 9, No. 7 (1934).
7. Sitterly, C. E. Moore - Private communication.
8. Glennon, B. M. and W.L. Wiese - Natl. Bur. Stds. Monograph 50 (1962).
9. Peterson, R. - Phys. and Chem. of Solids 1, 284 (1957).
10. Mandel'stam, S. L. - Space Science Reviews 4, 587 (1965).
11. Edlen, B. - Zeitschrift fur Physik 100, 726 (1936).
12. Ferner, E. - Ark. Mat. Astr. Fys. (Stockholm) 36A, 1 (1948).
13. Pecker, C. and F. Rohrllich - Astrophys. Jour. Supplement 8, 227 (1963).
14. Jordan, C. - Communications from University of London Observatory, No. 68 (1965).
15. Gold, A. and R. S. Knox - Physical Review 113, 834 (1959).
16. Korolev, F. A. and V. I. Odintsov, and E. V. Fursova - Optics and Spectroscopy 16, 304 (1964).